Dynamical picture of spin Hall effect based on quantum spin vorticity theory

AUTHOR(S):

Fukuda, Masahiro; Ichikawa, Kazuhide; Senami, Masato; Tachibana, Akitomo

CITATION:

Fukuda, Masahiro ...[et al]. Dynamical picture of spin Hall effect based on quantum spin vorticity theory. AIP Advances 2016, 6: 025108.

ISSUE DATE:

2016-02-01

URL:

http://hdl.handle.net/2433/218459

Dynamical picture of spin Hall effect based on quantum spin vorticity theory

Masahiro Fukuda, Kazuhide Ichikawa, Masato Senami, and Akitomo Tachibana

Citation: AIP Advances **6**, 025108 (2016); doi: 10.1063/1.4942087
View online: http://dx.doi.org/10.1063/1.4942087
View Table of Contents: http://aip.scitation.org/toc/adv/6/2
Published by the American Institute of Physics

AIP ADVANCES **6**, 025108 (2016)

Dynamical picture of spin Hall effect based on quantum spin vorticity theory

Masahiro Fukuda, Kazuhide Ichikawa, Masato Senami, and Akitomo Tachibana[a]
Department of Micro Engineering, Kyoto University, Kyoto 615-8540, Japan

(Received 9 November 2015; accepted 3 February 2016; published online 11 February 2016)

It is proposed that the dynamical picture of the spin Hall effect can be explained as the generation of the spin vorticity by the applied electric field on the basis of the "quantum spin vorticity theory", which describes the equation of motion of local spin and the vorticity of spin in the framework of quantum field theory. Similarly, it is proposed that the dynamical picture of the inverse spin Hall effect can be explained as the acceleration of the electron by the rotation of the spin torque density as driving force accompanying the generation of the spin vorticity. These explanations may help us to understand spin phenomena in condensed matter and molecular systems from a unified viewpoint. [http://dx.doi.org/10.1063/1.4942087]

I. INTRODUCTION

The spin Hall effect (SHE), which refers to a conversion of an electric current into a transverse flow of spin, is one of the most important phenomena in the field of spintronics. Historically, the SHE was predicted theoretically first,[1] and later experimental observations were performed in various types of materials by novel technology. The SHE was proposed theoretically as an analogue of the anomalous Hall effect.[2] Early proposed theories for the SHE are the so-called extrinsic mechanisms, which are based on the spin dependent scattering of electrons by impurities.[1,3] Later, the intrinsic mechanism of the SHE in a semiconductor system was proposed on the basis of the concept of dissipationless quantum spin currents.[4,5] Although theoretical discussion about the origin of the SHE still continues, many experiments show the SHE is an observable physical phenomenon. The first experimental observation of the SHE in a semiconductor was performed by Kato *et al*.[6] They detected electrically induced spin accumulation near the edges of the semiconductor by using Kerr rotation microscopy. Subsequently, Wunderlich *et al*. demonstrated the SHE by detecting circularly polarized light emitted from a light-emitting diode structure.[7] Furthermore, observations of the SHE in a metallic conductor,[8,9] and the inverse SHE (ISHE),[10,11] have been already reported. As for the theoretical side, an effective theory for spin-Hall effect not only in insulating but on equal footing also in conducting state by using a fully relativistic but model Hamiltonian has been discussed.[12]

So far, the SHE has been treated by using the concept of the spin current. Even if the idea of the spin current is suitable to analyze application devices, it is insufficient to understand spin dynamical phenomena from the viewpoint of fundamental physics. Namely, it is significant to understand such phenomena by dynamical pictures depicted with quantities derived from the symmetric energy-momentum tensor. From this point of view, in this study, we discuss theoretical aspects of the SHE and ISHE on the basis of a more fundamental theory called the "quantum spin vorticity theory",[13–17] which can give physical dynamical quantities as local quantities. While quantum mechanics cannot explain local contribution due to the definition of the inner product, which is derived by the integration over the whole region, quantum field theory can give the definition of local physical quantities without losing local contributions. Therefore, the quantum spin vorticity theory

[a]Electronic mail: akitomo@scl.kyoto-u.ac.jp

gives the equation of motion of local spin and the equation for the vorticity of the spin without losing local contributions. In particular, the "spin vorticity", which is a local quantity defined as the rotation of the spin angular momentum density, is neglected in the framework of quantum mechanics. On the other hand, the quantum spin vorticity theory reveals that the spin vorticity is crucial for investigating spin dynamics as a component of the local momentum density. The spin vorticity helps us to understand spin phenomena in molecular systems and even in condensed matter systems from a unified viewpoint.

In this paper, firstly we review the quantum spin vorticity theory. After we explain the local physical quantities, which are defined in quantum field theory, we show numerical calculation results of the local physical quantities in a simple carbon chain under a bias voltage as a demonstration. For these calculations of the local physical quantities defined by quantum field theory, we use a quantum mechanical wave packet by the non-equilibrium Green's function method as an approximation to a quantum field theoretical one. Finally, we show the SHE and ISHE can be explained by a local dynamical picture without introducing the spin current but with the spin vorticity.

II. QUANTUM SPIN VORTICITY THEORY

First of all, we review the quantum spin vorticity theory. In this paper, we discuss this theory in the framework of general relativity, though it can be applied even in the framework of supergravity.[16] In general relativity, the energy-momentum tensor obtained from the variational principle with a Lagrangian which is invariant under the general coordinate transformation must be a symmetric tensor. This requirement leads to the equation of spin dynamics, which reveals an important role of the spin vorticity for spin dynamics in the limit to the Minkowski space-time. We begin by introducing the Lagrangian density $\hat{L}$ for the quantum electrodynamics system with an electromagnetic field under external gravity. The Lagrangian density $\hat{L}$ is written as the sum of the Lagrangian density of the electron $\hat{L}_e$ and that of the electromagnetic field $\hat{L}_{\rm EM}$,

$$\hat{L}_e = \frac{c}{2}\left(\hat{\bar{\psi}}(i\hbar\gamma^a e_a{}^{\mu}\hat{D}_{e\mu}(g) - m_e c)\hat{\psi} + h.c.\right), \quad \hat{L}_{EM} = -\frac{1}{16\pi}\hat{F}_{\mu\nu}\hat{F}_{\rho\sigma}g^{\mu\rho}g^{\nu\sigma}, \tag{1}$$

where $\hat{\psi}$ denotes the Dirac spinor of the electron, $\hat{\bar{\psi}} = \hat{\psi}^{\dagger}\gamma^0$, γ^a are Dirac gamma matrices, $e_a{}^{\mu}$ is the tetrad field, m_e is the electron mass, c is the speed of light in vacuum, and $g^{\mu\nu}$ is the metric tensor. The electromagnetic field strength tensor is $\hat{F}_{\mu\nu} = \partial_\mu\hat{A}_\nu - \partial_\nu\hat{A}_\mu$, where $\hat{A}_\mu$ is the gauge field. Here, Greek indices and Latin indices from a to d run over 0 to 3. The former refers to the general coordinate indices, while the latter refers to the local Lorentz frame indices. We adopt the Einstein summation convention. The gravitational covariant derivative is written as

$$\hat{D}_{e\mu}(g) = \hat{D}_{e\mu} + i\frac{1}{2\hbar}\gamma_{ab\mu}J^{ab}, \quad \hat{D}_{e\mu} = \partial_\mu + i\frac{Z_e e}{\hbar c}\hat{A}_\mu, \tag{2}$$

where $\hat{D}_{e\mu}$ is the gauge covariant derivative, $J^{ab} = \frac{i\hbar}{4}\left[\gamma^a, \gamma^b\right]$, $\gamma_{ab\mu}$ is the spin connection,[18] e is the electron charge ($e > 0$) and $Z_e = -1$. The variational principle for the system action with respect to the tetrad field leads to the symmetric energy-momentum tensor $T_{\mu\nu}$ as follows[19]:

$$\hat{T}_{\mu\nu} = \frac{1}{\sqrt{-g}}\eta_{ab}e^b{}_\nu\frac{\delta\left(\hat{L}\sqrt{-g}\right)}{\delta e_a{}^{\mu}} = \hat{T}_{e\mu\nu} + \hat{T}_{\mathrm{EM}\mu\nu}. \tag{3}$$

Writing the right-hand side explicitly,

$$\hat{T}_{e\mu\nu} = -\hat{\varepsilon}^{\Pi}_{\mu\nu} - \hat{\tau}^{\Pi}_{e\mu\nu}(g) - g_{\mu\nu}\hat{L}_e = \hat{T}_{e\nu\mu}, \tag{4}$$

$$\hat{\varepsilon}^{\Pi}_{\mu\nu} = -\frac{1}{\sqrt{-g}}\eta_{ab}e^b{}_\nu\left[\frac{\partial\left(\hat{L}_e\sqrt{-g}\right)}{\partial\gamma^{cd}{}_\rho}\frac{\partial\gamma^{cd}{}_\rho}{\partial e_a{}^\mu} - \partial_\sigma\left(\frac{\partial\left(\hat{L}_e\sqrt{-g}\right)}{\partial\gamma^{cd}{}_\rho}\frac{\partial\gamma^{cd}{}_\rho}{\partial\left(\partial_\sigma e_a{}^\mu\right)}\right)\right], \tag{5}$$

$$\hat{\tau}^{\Pi}_{e\mu\nu}(g) = -\frac{1}{\sqrt{-g}}\eta_{ab}e^b{}_\nu\frac{\partial\left(\hat{L}_e\sqrt{-g}\right)}{\partial e_a{}^\mu} = \frac{c}{2}\left(\hat{\psi}^\dagger\gamma^0\gamma_\nu\left(-i\hbar\hat{D}_\mu(g)\right)\hat{\psi} + h.c.\right), \tag{6}$$

$$\hat{T}_{\mathrm{EM}\mu\nu} = -\frac{1}{4\pi} g^{\rho\sigma} \hat{F}_{\mu\rho} \hat{F}_{\nu\sigma} - g_{\mu\nu} \hat{L}_{\mathrm{EM}} = \hat{T}_{\mathrm{EM}\nu\mu}, \tag{7}$$

where $g = \det g_{\mu\nu}$ and $\eta_{\mu\nu} = \mathrm{diag}(1,-1,-1,-1) = \eta^{\mu\nu}$. The concrete expression of Eq. (5) is written in Ref. 13. Note that $\hat{\varepsilon}^{\Pi}_{\mu\nu}$ and $\hat{\tau}^{\Pi}_{e\mu\nu}(g)$ are not necessarily symmetric tensors. To emphasize this, we put the superscript Π and call them symmetry-polarized geometrical tensor and symmetry-polarized electronic stress tensor, respectively.[13] These tensors can be decomposed into a symmetric part and an anti-symmetric part as $\hat{\varepsilon}^{\Pi\mu\nu} = \hat{\varepsilon}^{S\mu\nu} + \hat{\varepsilon}^{A\mu\nu}$ and $\hat{\tau}_e^{\Pi\mu\nu}(g) = \hat{\tau}_e^{S\mu\nu}(g) + \hat{\tau}_e^{A\mu\nu}(g)$.

Since the energy-momentum tensor is symmetric, the anti-symmetric parts $\hat{\varepsilon}^{A}_{\mu\nu}$ and $\hat{\tau}^{A}_{e\mu\nu}$ cancel with each other:

$$\hat{\varepsilon}^{A\mu\nu} + \hat{\tau}_e^{A\mu\nu}(g) = 0. \tag{8}$$

Eq. (8) is called the quantum spin vorticity principle. In the limit to the Minkowski space-time, it is revealed that Eq. (8) describes spin dynamics. In the limit of $e^a{}_\mu \to \delta^a{}_\mu$ and $g_{\mu\nu} \to \eta_{\mu\nu}$, the symmetric energy-momentum tensors $\hat{T}_e^{\mu\nu}$ and $\hat{T}_{\mathrm{EM}}^{\mu\nu}$ are reduced to

$$\hat{T}_e^{\mu\nu} = -\hat{\varepsilon}^{\Pi\mu\nu} - \hat{\tau}_e^{\Pi\mu\nu} - \eta^{\mu\nu}\hat{L}_e, \quad \hat{T}_{\mathrm{EM}}^{\mu\nu} = -\frac{1}{4\pi}\eta^{\rho\sigma}\hat{F}^{\mu}{}_{\rho}\hat{F}^{\nu}{}_{\sigma} - \eta^{\mu\nu}\hat{L}_{EM}, \tag{9}$$

$$\hat{\varepsilon}^{\Pi\mu\nu} = -\frac{\hbar}{4Z_e e}\epsilon^{\mu\nu\lambda\sigma}\partial_\lambda \hat{j}_{5\sigma}, \quad \hat{\tau}_e^{\Pi\mu\nu} = \frac{c}{2}\left(\hat{\psi}^\dagger\gamma^0\gamma^\nu\left(-i\hbar\hat{D}_e^\mu\right)\hat{\psi} + h.c.\right), \tag{10}$$

where $\epsilon^{\mu\nu\lambda\sigma}$ is the Levi-Civita tensor, $\hat{j}_5^\mu = Z_e ec\hat{\bar{\psi}}\gamma^\mu\gamma_5\hat{\psi}$ is the chiral current and $\gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3$. Then, Eq. (8) is also reduced to the following equations:

$$\frac{\partial}{\partial t}\hat{\vec{s}}_e = \hat{\vec{t}}_e + \hat{\vec{\zeta}}_e, \tag{11}$$

$$\mathrm{rot}\hat{\vec{s}}_e = \frac{1}{2}\left(\hat{\bar{\psi}}\vec{\gamma}\left(i\hbar\hat{D}_{e0}\right)\hat{\psi} + h.c.\right) - \hat{\vec{\Pi}}_e, \tag{12}$$

where the spin angular momentum density $\hat{\vec{s}}_e$, the spin torque density $\hat{\vec{t}}_e$, the zeta force density $\hat{\vec{\zeta}}_e$, and the kinetic momentum density $\hat{\vec{\Pi}}_e$ are defined as

$$\hat{s}_e^i = \hat{\psi}^\dagger\frac{\hbar}{2}\Sigma^i\hat{\psi} = \frac{\hbar}{2Z_e ec}\hat{j}_5^i, \quad \hat{t}_e^i = -\epsilon_{ijk}\hat{\tau}_e^{Ajk}, \tag{13}$$

$$\hat{\zeta}_e^i = -\partial_i\hat{\phi}_5, \quad \hat{\phi}_5 = \frac{\hbar}{2Z_e e}\hat{j}_5^0, \quad \hat{\Pi}_e^i = \frac{1}{2}\left(\hat{\bar{\psi}}\gamma^0\left(i\hbar\hat{D}_e^i\right)\hat{\psi} + h.c.\right). \tag{14}$$

In the equations above, Σ^i is the 4×4 Pauli matrix, and ϵ_{ijk} is the Levi-Civita tensor. Hereafter, Latin letters run from 1 to 3. As are clear from the above definitions, these operators are expressed by using the field operators of the electron $\hat{\psi}$ and the photon $\hat{A}^\mu$. The physical quantities are given as expectation values for a time-independent state vector in the Heisenberg picture such as $O = \langle\Phi|\hat{O}|\Phi\rangle - \langle 0|\hat{O}|0\rangle$. Actual effects of condensed matter, which may break some symmetry, are included in the state vector.

Apparently, Eq. (11) and Eq. (12) are the equation of motion of the spin angular momentum density and the equation for the vorticity of spin, respectively. We note that Eqs. (11) and (12) are related to the angular momentum and momentum, respectively. The equation of motion of spin angular momentum density shown in Eq. (11) is derived in the framework of quantum field theory, and hence it does not average out the local contribution, while the Heisenberg equation in relativistic quantum mechanics[20] cannot describe local spin dynamics since a physical quantity in quantum mechanics is defined by the inner product, which is derived by the integration over the whole region. The zeta force density does not appear in the equation of motion of spin in the framework of relativistic quantum mechanics. In present experimental apparatuses, the local effect of the zeta force density is integrated into a small surface effect, so that it has not been observed experimentally yet. For example, the details of the spin torque and the zeta force for atomic and molecular systems were discussed in Refs. 21–23.

Let us now focus on Eq. (12). It implies that the vorticity of the electronic spin contributes to the momentum of the electron. We can see the fact clearly from the expression of the electronic momentum density $\hat{P}_e^i = \frac{1}{c}\hat{T}_e^{i0}$, which includes half of the spin vorticity as follows[14]:

$$\hat{\vec{P}}_e = \hat{\vec{\Pi}}_e + \frac{1}{2}\mathrm{rot}\hat{\vec{s}}_e. \tag{15}$$

Although the second term, which is the contribution from spin, as well as the zeta force density disappears after integration over the whole of space, its contribution cannot be neglected in a local region. In other words, the electronic momentum density, which is derived by the covariant symmetry of the general coordinate transformation, includes the local contribution of half of the spin vorticity unlike the definition of the momentum in quantum mechanics. Furthermore, the time derivative of the electronic momentum density is given as

$$\frac{\partial}{\partial t}\hat{\vec{P}}_e = \hat{\vec{L}}_e + \hat{\vec{\tau}}_e{}^S, \tag{16}$$

where $\hat{\vec{L}}_e = \hat{\vec{E}}\hat{j}_e^0 + \frac{1}{c}\hat{\vec{j}}_e \times \hat{\vec{B}}$ is the Lorentz force density, $\hat{j}_e^\mu = Z_e ec\hat{\bar{\psi}}\gamma^\mu\hat{\psi}$ is the electronic charge current density, $\hat{\vec{E}} = -\mathrm{grad}\hat{A}_0 - \frac{1}{c}\frac{\partial\hat{\vec{A}}}{\partial t}$ is the electric field and $\hat{\vec{B}} = \mathrm{rot}\hat{\vec{A}}$ is the magnetic field. The second term on the right-hand side, $\hat{\vec{\tau}}_e{}^S = \mathrm{div}\hat{\overleftrightarrow{\tau}}_e{}^S$, is the tension density,[24,25] which is defined as the divergence of the symmetric parts of the electronic stress tensor $\hat{\overleftrightarrow{\tau}}_e{}^S$. Since the tension density as well as the spin vorticity disappears after integrating over the whole region, the above equation is reduced to $\frac{\partial}{\partial t}\int \hat{\vec{\Pi}}_e d^3\vec{r} = \int \hat{\vec{L}}_e d^3\vec{r}$, which is a well known equation of motion in the framework of relativistic quantum mechanics.[20] By using Eq. (11), the time derivative of half of the spin vorticity is given easily as follows:

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\mathrm{rot}\,\hat{\vec{s}}_e\right) = \frac{1}{2}\mathrm{rot}\,\hat{\vec{t}}_e = -\,\mathrm{div}\hat{\overleftrightarrow{\tau}}_e{}^A. \tag{17}$$

This means that the divergence of the anti-symmetric part of the stress tensor $\hat{\overleftrightarrow{\tau}}_e{}^A$ generates spin vorticity. By using Eq. (17), Eq. (16) can be rewritten as

$$\frac{\partial}{\partial t}\hat{\vec{\Pi}}_e = \hat{\vec{L}}_e + \hat{\vec{\tau}}_e{}^S - \frac{1}{2}\mathrm{rot}\,\hat{\vec{t}}_e. \tag{18}$$

Equations (17) and (18) express that the rotation of the spin torque density $\hat{\vec{t}}_e$ as driving force generates the kinetic momentum density $\hat{\vec{\Pi}}_e$ accompanying the generation of half of the spin vorticity, $\frac{1}{2}\mathrm{rot}\hat{\vec{s}}_e$. This interpretation is a consequence of the quantum spin vorticity theory.

Thus, in the spin vorticity theory, the equations regarding operators of the physical quantities derived from the energy-momentum tensor are discussed. When we calculate a physical quantity, we need both the operator of the physical quantity and the state vector of quantum field theory. The equations of operators discussed in the spin vorticity theory can be applied to QED systems universally, though the validity of the result of the physical quantity depends on how the state vector of the system is calculated.

III. NUMERICAL CALCULATIONS OF SPIN VORTICITY

As an application example of the quantum spin vorticity theory, we demonstrate the generation of the spin vorticity in a local region by using a simple carbon chain, attaching both edges to electrodes in the presence of a finite bias voltage. The carbon chain is one of the ideal model systems for studying the electronic structure under a bias voltage and is also applicable in molecular device design as one of the nano carbon systems (such as rings, fullerenes, and graphenes). Therefore, the carbon chain is suitable for our first demonstration to understand spin phenomena in condensed matter and molecular systems from a unified viewpoint. Although, rigorously speaking, the electronic bound state of quantum field theory is required for calculations of the local physical quantities, such a calculation method is not established for our purpose at this moment. (Incidentally, we are trying to develop a program code *QEDynamics*[28] to calculate the electronic state described by quantum field theory, but this is still work in progress.) Therefore, we use a relativistic quantum mechanical wave packet as an approximation to the state vector of quantum field theory in order to calculate the local physical quantities, which are given as the expectation values of the density operators defined by quantum field theory. Nevertheless, it is sufficient to grasp some aspects of the spin vorticity. This wave packet in the steady state of the system is given by an *ab initio* calculation based on density-functional theory (DFT). Although this system is not dynamical, the local picture in the nonequilibrium state can be demonstrated. The electronic structure is calculated by means of a non-equilibrium Green's function method[29,30] coupled with a local spin density approximation[31] in density-functional theory.[32] Since this method is widely used for calculations of spin densities induced by a bias voltage,[33] it is suitable to demonstrate the distribution calculation of the local physical quantities such as the spin vorticity. All of the calculations were performed by an *ab initio* DFT code, OPENMX.[34,33] We made some modifications to the program code for our purpose of calculating local physical quantities, which are calculated by using the 2-component relativistic wave function as a substitute for the large component of the 4-component relativistic wave function. The electronic structure of a straight carbon chain with bond length of 1.5 Å under a finite bias voltage of 0.1 V is self-consistently determined under an electronic temperature of 300 K. Pseudoatomic orbitals centered on atomic sites are used as the basis function set.[35] We use the pseudoatomic orbitals specified by C5.0-$s2p2d1$, where C stands for the atomic symbol, 5.0 represents the cutoff radius (bohr), and $s2p2d1$ means the employment of two, two, and one orbitals for the s, p, and d component, respectively. The cutoff energy is set to 180 Ryd. The system we use consists of left and right electrodes and a central region. The electrodes are made of semi-infinite carbon chains and the central region contains eighteen carbon atoms.

The results are shown in FIG. 1. The kinetic momentum density, the spin angular momentum density and the spin vorticity of the system without bias voltage are smaller by two digits than those with the bias voltage 0.1 V. Hence, we only show the local physical quantities in the presence of the bias voltage 0.1 V in FIG. 1. Local physical quantities around six atoms in the center of the system, where the attaching electrodes have little direct effect, are shown in FIGs. 1(a), 1(c) and 1(e). FIGs. 1(b) and 1(d) show local physical quantities around a nucleus on a plane perpendicular to the carbon chain. The kinetic momentum density $\vec{\Pi}_e(\vec{r})$ is distributed along the π-bondings (FIG. 1(a)). On the other hand, we can see the spin angular momentum density $\vec{s}_e(\vec{r})$ is distributed circularly around the nuclei (FIGs. 1(c) and 1(d)), and therefore, the spin vorticity $\mathrm{rot}\vec{s}_e(\vec{r})$ is concentrated around a nucleus (FIG. 1(e)). The distribution of the spin angular momentum density on the cross

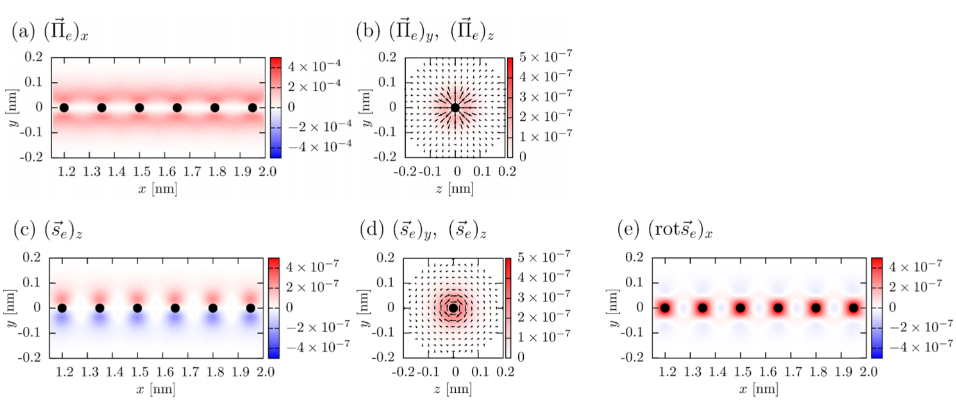

FIG. 1. (a) The distributions of the x component of the kinetic momentum density on the plane $z = 0$ [nm], and (b) y and z components on the plane $x = 1.65$ [nm]. (c) The distributions of the z component of the spin angular momentum density on the plane $z = 0$ [nm], and (d) y and z components on the plane $x = 1.65$ [nm]. (e) The distribution of the x component of the spin vorticity on the plane $z = 0$ [nm]. The y and z components of the spin vorticity on the plane $z = 0$ [nm] are negligibly small. In panels (b) and (d), the vectors consist of y and z components, and the color maps represent the norm of the vectors.

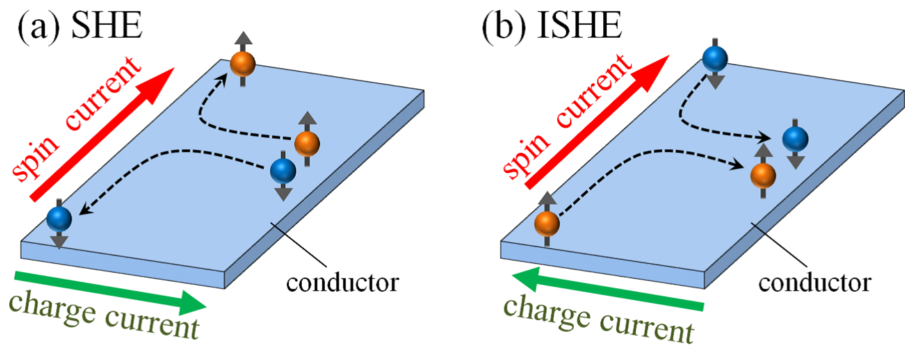

FIG. 2. Conventional concepts of SHE and ISHE. (a) The SHE is understood as a conversion of a charge current into a transverse spin current. (b) The ISHE is understood as a conversion of an injected spin current into a transverse charge current.

section shown in FIG. 1(c) is similar to spin accumulation on a flat device which is observed experimentally as the SHE. However, in case of the carbon chain, the spin angular momentum density forms clear vortices because of the rotational symmetry of the system.

IV. APPLICATION TO THE SPIN HALL EFFECT

Finally, we propose a new dynamical picture of the SHE based on the spin vorticity theory. The conventional SHE refers to the conversion of a charge current into a transverse spin current due to the spin-orbit interaction [see Fig. 2(a)]. Although definitions of the spin current are discussed in Ref. 26, it is actually almost impossible to observe the spin current directly by electromagnetic detection. Furthermore, the relation between spin currents and observable physical quantities such as spin accumulation is unclear. This is because total spin is not conserved in general due to for example spin damping by spin-orbit interactions.[27] However, in the quantum spin vorticity theory, the dynamical picture of the SHE is not dependent on the concept of the spin current. Alternatively, the spin transfer can be explained by the time evolution of the spin vorticity without invoking the spin current. Half of the spin vorticity is introduced naturally as a component of the electron momentum density on the basis of the quantum spin vorticity theory as mentioned above. In addition, the spin vorticity is an observable local physical quantity in principle and actually can be measured experimentally by the distribution of the spin angular momentum density for a system with large scale spin distribution such as the SHE, since the spin vorticity is defined as the rotation of the spin angular momentum density.

After all, the SHE is described by using the spin vorticity as follows. When the electric field is given in a conductor, the Lorentz force density $\vec{L}_e$ is generated. The Lorentz force density increases the total electronic momentum density $\vec{P}_e$, which consists of the kinetic momentum density $\vec{\Pi}_e$ and half of the spin vorticity $\frac{1}{2}\mathrm{rot}\vec{s}_e$ (see Eqs. (15) and (16)). The degree of the assignment of $\vec{P}_e$ to $\vec{\Pi}_e$ and $\frac{1}{2}\mathrm{rot}\vec{s}_e$ depends on the divergence of the anti-symmetric stress tensor $\overleftrightarrow{\tau}_e^{\,A}$ at each point in space-time (see Eqs. (17) and (18)). Since the anti-symmetric stress tensor is zero in the non-relativistic limit, the relativistic interaction is necessary for the generation of the spin vorticity. Therefore, the spin vorticity is generated mainly around nuclei (or impurities), where the relativistic interaction is strong in the conductor. In addition, the superposition of the spin vorticity causes accumulation of spin at both edges of the conductor [see Fig. 3(a)]. Similarly, although the conventional ISHE refers to the conversion of an injected spin current into a transverse charge current or voltage [see Fig. 2(b)], this phenomenon is described by using the electron spin vorticity theory as follows. When the rotation of the spin torque density is given in a conductor, the distribution of the spin angular momentum density becomes non-uniform, and it generates the spin vorticity (see Eq. (17)). According to Eq. (18), the rotation of the spin torque also accelerates the electron, and it generates the kinetic momentum density [see Fig. 3(b)]. The degree of the generation of half of the spin vorticity and the kinetic momentum density depends on the divergence of the anti-symmetric

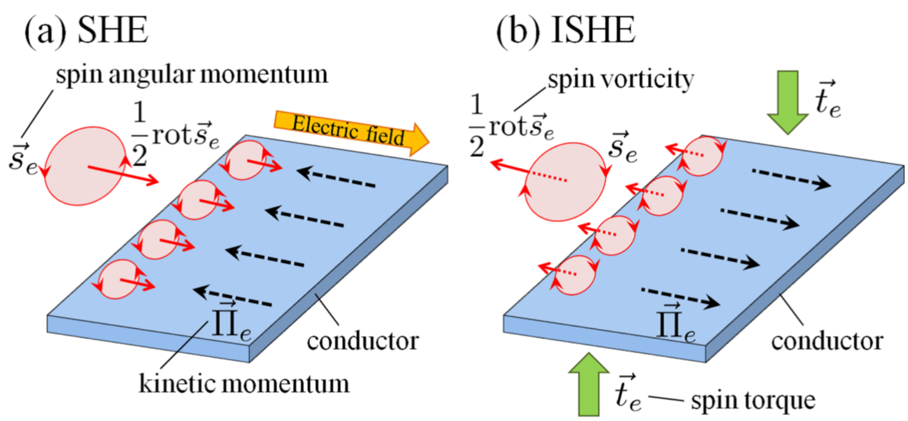

FIG. 3. Concept based on the quantum spin vorticity theory. (a) The SHE is understood as the generation of the spin vorticity by the applied electric field. (b) The ISHE is understood as the acceleration of the electron by the rotation of the spin torque density as driving force accompanying the generation of half of the spin vorticity.

stress tensor $\overleftrightarrow{\tau}_e^{\,A}$ at each point in space-time (see Eqs. (17) and (18)). Of course, the value and direction of the spin vorticity induced by a bias voltage depend on the species of nuclei and structures. Therefore, we will try to evaluate local physical quantities of more complex structures which are used in the fields of spintronics and multiferroics in our near future work.

V. CONCLUSIONS

In this paper, we have proposed the dynamical local picture of the spin Hall effect based on the quantum spin vorticity principle. In the quantum spin vorticity principle, half of the spin vorticity is introduced naturally as a component of the electron momentum density. We have performed numerical calculations of the local distributions of the kinetic momentum density and the spin vorticity induced by a finite bias voltage by using a relativistic quantum mechanical wave packet as an approximation to the state vector of the quantum field theory. We also proposed new dynamical pictures of the SHE and ISHE based on the quantum spin vorticity theory. The SHE is described as *the generation of the spin vorticity by the applied electric field in a conductor.* The ISHE is described as *the acceleration of the electron by the rotation of the spin torque density as driving force accompanying the generation of the spin vorticity in a conductor.* The spin vorticity will be a key to give unified understanding of physical phenomena related to spin in condensed matter and molecular systems beyond the field of spintronics.

ACKNOWLEDGMENTS

We thank Prof. Salam for helpful comments. This work was supported by a Grant-in-Aid for Scientific Research (25410012), a Grant-in-Aid for JSPS Fellows, and Toyota Physical and Chemical Research Institute Scholars.

[1] M. I. Dyakonov and V. I. Perel, JETP Lett. **13**, 467 (1971); Phys. Lett. **A35**, 459 (1971).
[2] N. Nagaosa, J. Sinova, S. Onoda, A. H. MacDonald, and N. P. Ong, Rev. Mod. Phys. **82**, 1539 (2010).
[3] J. E. Hirsch, Phys. Rev. Lett. **83**, 1834 (1999).
[4] S. Murakami, N. Nagaosa, and S.-C. Zhang, Science **301**, 1348 (2003).
[5] J. Sinova, D. Culcer, Q. Niu, N. A. Sinitsyn, T. Jungwirth, and A. H. MacDonald, Phys. Rev. Lett. **92**, 126603 (2004).
[6] Y. K. Kato, R. C. Myers, A. C. Gossard, and D. D. Awschalom, Science **306**, 1910 (2004).
[7] J. Wunderlich, B. Kaestner, J. Sinova, and T. Jungwirth, Phys. Rev. Lett. **94**, 047204 (2005).
[8] S. O. Valenzuela and M. Tinkham, Nature **442**, 176-179 (2007).
[9] T. Kimura, Y. Otani, T. Sato, S. Takahashi, and S. Maekawa, Phys. Rev. Lett. **98**, 156601 (2007).
[10] E. Saitoh, M. Ueda, H. Miyajima, and G. Tatara, Appl. Phys. Lett. **88**, 182509 (2006).
[11] K. Ando and E. Saitoh, Nat. Commun. **3**, 629 (2012).
[12] Y. Fuseya, M. Ogata, and H. Fukuyama, J. Phys. Soc. Jpn. **81**, 093704 (2012).

[13] A. Tachibana, J. Math. Chem. **50**, 669 (2012).
[14] A. Tachibana, "Electronic stress with spin vorticity," in *Concepts and Methods in Modern Theoretical Chemistry*, edited by S. K. Ghosh and P. K. Chattaraj (CRC Press, Florida, 2013), pp. 235–251.
[15] A. Tachibana, J. Comput. Chem. Jpn. **13**, 18 (2014).
[16] A. Tachibana, Indian J. Chem. A **53**, 1031 (2014).
[17] A. Tachibana, J. Math. Chem. **53**, 1943 (2015).
[18] S. Weinberg, *Quantum Theory of Fields III* (Cambridge University, Cambridge, 1995).
[19] S. Weinberg, *Gravitation and Cosmology: Principles and Applications of the General Theory of Relativity* (Wiley, New York, 1972).
[20] For example, see, A. Messiah, *Quantum Mechanics* (North-Holland, New York, 1961).
[21] M. Senami, J. Nishikawa, T. Hara, and A. Tachibana, J. Phys. Soc. Jpn **79**, 084302 (2010).
[22] T. Hara, M. Senami, and A. Tachibana, Phys. Lett. A. **376**, 1434 (2012).
[23] M. Fukuda, M. Senami, and A. Tachibana, in *Progress in Theoretical Chemistry and Physics*, edited by M. Hotokka, E. J. Brandas, J. Maruani, and G. Delgado-Barrio (Springer, 2013), Vol. 27, Chapter 7, pp. 131–139.
[24] A. Tachibana, J. Chem. Phys. **115**, 3497 (2001).
[25] A. Tachibana, J. Mol. Struct. :(THEOCHEM) **943**, 138 (2010).
[26] *Spin Current*, edited by S. Maekawa, S. O. Valenzuela, E. Saitoh, and T. Kimura (Oxford University Press, 2012).
[27] A. Takeuchi, K. Hosono, and G. Tatara, Phys. Rev. B **81**, 144405 (2010).
[28] *QEDynamics*, M. Senami, K. Ichikawa, and A. Tachibana, http://www.tachibana.kues.kyoto-u.ac.jp/qed/.
[29] L. V. Keldysh, Sov. Phys. JETP **20**, 1018 (1965); C. Caroli, R. Combescot, P. Nozieres, and D. Saint-James, J. Phys. C **4**, 916 (1971).
[30] H. Kondo, H. Kino, J. Nara, T. Ozaki, and T. Ohno, Phys. Rev. B **73**, 235323 (2006).
[31] D. M. Ceperley and B. J. Alder, Phys. Rev. Lett. **45**, 566 (1980); J. P. Perdew and A. Zunger, Phys. Rev. B **23**, 5048 (1981).
[32] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964); W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).
[33] T. Ozaki, K. Nishio, and H. Kino, Phys. Rev. B **81**, 035116 (2010).
[34] T. Ozaki *et al.*, OpenMX package, http://www.openmx-square.org/.
[35] T. Ozaki, Phys. Rev. B **67**, 155108 (2003).